



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:51 PM UTC

PDB ID : 3TVU / pdb_00003tvu
Title : Crystal Structure of the humanized carboxyltransferase domain of yeast Acetyl-coA carboxylase in complex with compound 3
Authors : Rajamohan, F.; Marr, E.; Reyes, A.; Landro, J.A.; Anderson, M.D.; Corbett, J.W.; Dirico, K.J.; Harwood, J.H.; Tu, M.; Vajdos, F.F.
Deposited on : 2011-09-20
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

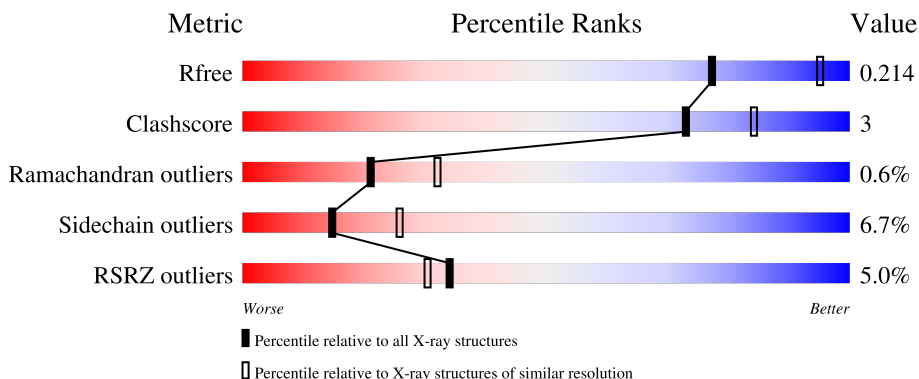
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	769	4% 77% 13% • 9%
1	B	769	5% 76% 12% • 10%
1	C	769	4% 74% 12% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17661 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	1	0
			5561	3539	960	1045	17			
1	B	690	Total	C	N	O	S	0	0	0
			5513	3510	949	1037	17			
1	C	681	Total	C	N	O	S	0	0	0
			5437	3454	939	1027	17			

There are 60 discrepancies between the modelled and reference sequences:

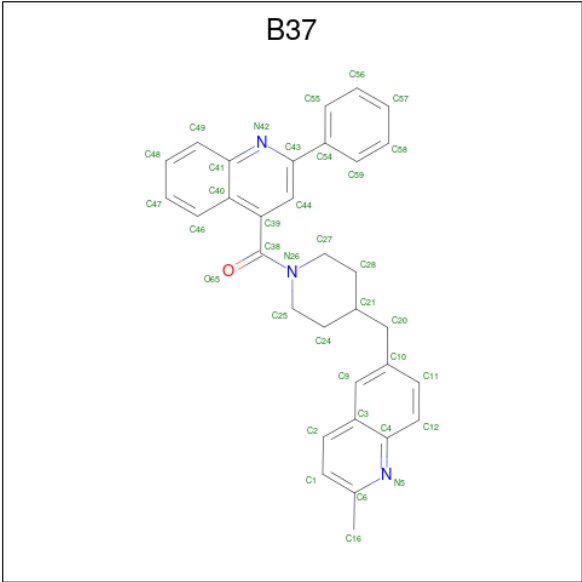
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	1760	SER	PRO	engineered mutation	UNP Q00955
A	1762	LEU	ILE	engineered mutation	UNP Q00955
A	1765	VAL	MET	engineered mutation	UNP Q00955
A	1919	GLN	GLU	engineered mutation	UNP Q00955
A	1920	ALA	PRO	engineered mutation	UNP Q00955
A	1925	PHE	HIS	engineered mutation	UNP Q00955
A	2028	GLU	GLN	engineered mutation	UNP Q00955
A	2030	THR	MET	engineered mutation	UNP Q00955
A	2032	GLU	GLY	engineered mutation	UNP Q00955
A	2234	LEU	-	expression tag	UNP Q00955
A	2235	GLU	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
A	2240	HIS	-	expression tag	UNP Q00955
A	2241	HIS	-	expression tag	UNP Q00955
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered mutation	UNP Q00955
B	2028	GLU	GLN	engineered mutation	UNP Q00955
B	2030	THR	MET	engineered mutation	UNP Q00955
B	2032	GLU	GLY	engineered mutation	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	1760	SER	PRO	engineered mutation	UNP Q00955
C	1762	LEU	ILE	engineered mutation	UNP Q00955
C	1765	VAL	MET	engineered mutation	UNP Q00955
C	1919	GLN	GLU	engineered mutation	UNP Q00955
C	1920	ALA	PRO	engineered mutation	UNP Q00955
C	1925	PHE	HIS	engineered mutation	UNP Q00955
C	2028	GLU	GLN	engineered mutation	UNP Q00955
C	2030	THR	MET	engineered mutation	UNP Q00955
C	2032	GLU	GLY	engineered mutation	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 4-({4-[(2-methylquinolin-6-yl)methyl]piperidin-1-yl}carbonyl)-2-phenylquinoline (CCD ID: B37) (formula: C₃₂H₂₉N₃O).

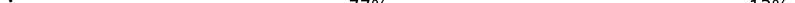


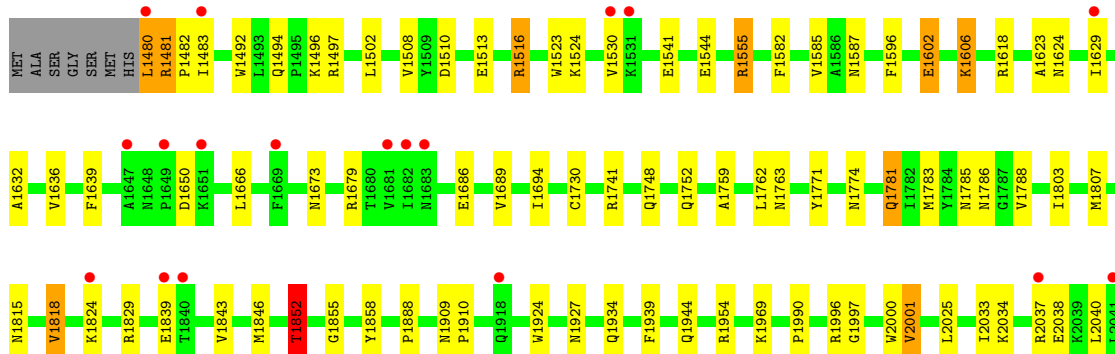
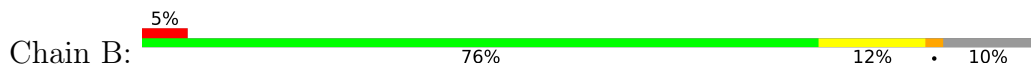
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	32	3	1		
2	B	1	Total	C	N	O	0	0
			36	32	3	1		
2	C	1	Total	C	N	O	0	0
			36	32	3	1		

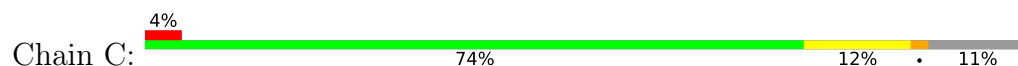
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	382	Total	O	0	0
			382	382		
3	B	339	Total	O	0	0
			339	339		
3	C	321	Total	O	0	0
			321	321		

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A:  4% 77% 13% 9%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.99Å 123.18Å 146.16Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	43.55 – 2.40 43.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.55-2.40) 96.4 (43.55-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.202 , 0.223 0.191 , 0.214	Depositor DCC
R_{free} test set	16364 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17661	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B37

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.85	0/5689	1.34	19/7704 (0.2%)
1	B	0.83	1/5633 (0.0%)	1.35	21/7631 (0.3%)
1	C	0.83	1/5551 (0.0%)	1.38	23/7512 (0.3%)
All	All	0.84	2/16873 (0.0%)	1.36	63/22847 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1636	VAL	CA-CB	5.02	1.56	1.54
1	C	1636	VAL	CA-CB	5.01	1.56	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2079	GLU	CA-C-N	10.03	139.75	121.70
1	C	2079	GLU	C-N-CA	10.03	139.75	121.70
1	B	2080	ARG	CA-C-N	9.92	139.56	121.70
1	B	2080	ARG	C-N-CA	9.92	139.56	121.70
1	C	2080	ARG	CA-C-N	8.49	136.99	121.70
1	C	2080	ARG	C-N-CA	8.49	136.99	121.70
1	A	1730	CYS	N-CA-C	-8.27	97.32	108.74
1	A	2191	LEU	N-CA-C	-7.55	103.15	112.88
1	C	1740	VAL	N-CA-CB	7.00	120.06	110.54
1	C	2152	ILE	N-CA-CB	6.82	120.81	110.58
1	A	1785	ASN	CA-C-N	6.69	132.06	120.68
1	A	1785	ASN	C-N-CA	6.69	132.06	120.68
1	B	2152	ILE	N-CA-CB	6.64	120.55	110.58
1	A	1596	PHE	CA-CB-CG	6.37	120.17	113.80
1	C	1596	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	1624	ASN	N-CA-C	6.17	117.25	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1785	ASN	CA-C-N	6.17	131.16	120.68
1	B	1785	ASN	C-N-CA	6.17	131.16	120.68
1	C	1624	ASN	N-CA-C	6.12	117.19	108.74
1	B	2037	ARG	N-CA-C	5.96	118.53	111.33
1	B	2001	VAL	N-CA-CB	5.86	117.80	110.47
1	B	2080	ARG	N-CA-C	5.84	118.53	111.40
1	C	2079	GLU	CA-C-O	-5.84	114.19	121.02
1	C	2148	ARG	CA-C-N	5.78	128.03	120.28
1	C	2148	ARG	C-N-CA	5.78	128.03	120.28
1	B	1624	ASN	N-CA-C	5.76	116.68	108.74
1	B	1786	ASN	CB-CA-C	-5.75	98.65	110.38
1	B	1939	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	1803	ILE	CA-C-N	5.70	128.27	120.46
1	B	1803	ILE	C-N-CA	5.70	128.27	120.46
1	B	1596	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	2001	VAL	CA-C-N	5.61	130.11	121.19
1	A	2001	VAL	C-N-CA	5.61	130.11	121.19
1	B	1852	THR	CB-CA-C	5.59	120.51	109.66
1	C	1650	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	1650	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	2001	VAL	N-CA-CB	5.53	117.39	110.47
1	C	1792	THR	CB-CA-C	5.49	120.14	109.33
1	C	1645	ASP	CA-CB-CG	5.47	118.08	112.60
1	B	1927	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	1927	ASN	CA-CB-CG	5.43	118.03	112.60
1	B	2172	ALA	CA-C-N	5.42	127.49	120.44
1	B	2172	ALA	C-N-CA	5.42	127.49	120.44
1	C	2052	ARG	CA-C-N	5.34	127.69	120.38
1	C	2052	ARG	C-N-CA	5.34	127.69	120.38
1	A	1783	MET	N-CA-C	5.33	118.00	111.82
1	B	1818	VAL	CB-CA-C	5.29	116.06	110.88
1	A	1973	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	2145	GLU	N-CA-C	5.28	116.67	107.49
1	A	1803	ILE	CA-C-N	5.27	127.68	120.46
1	A	1803	ILE	C-N-CA	5.27	127.68	120.46
1	C	2001	VAL	N-CA-C	5.27	116.63	110.62
1	A	1939	PHE	CA-CB-CG	5.26	119.06	113.80
1	C	1545	ASP	CA-C-N	5.25	127.57	120.38
1	C	1545	ASP	C-N-CA	5.25	127.57	120.38
1	C	1973	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	1939	PHE	CA-CB-CG	5.16	118.95	113.80
1	C	1927	ASN	CA-CB-CG	5.13	117.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1788	VAL	N-CA-C	-5.11	105.56	110.72
1	A	1729	THR	CA-C-N	5.10	130.22	122.11
1	A	1729	THR	C-N-CA	5.10	130.22	122.11
1	B	1788	VAL	N-CA-C	-5.09	105.57	110.72
1	A	2034	LYS	N-CA-C	5.06	120.29	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5561	0	5492	33	0
1	B	5513	0	5450	42	0
1	C	5437	0	5373	39	0
2	A	36	0	29	0	0
2	B	36	0	29	0	0
2	C	36	0	29	0	0
3	A	382	0	0	3	0
3	B	339	0	0	0	0
3	C	321	0	0	3	0
All	All	17661	0	16402	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.18	0.88
1:C:1815:ASN:H	1:C:1944:GLN:HE22	1.21	0.86
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.22	0.84
1:A:1763:ASN:HD21	1:A:1771:TYR:H	1.24	0.84
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.19	0.84
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1632:ALA:H	1:C:2097:HIS:HE1	1.30	0.78
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.86	0.76
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.38	0.72
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.25	0.69
1:A:1877:VAL:HG23	1:A:1928:SER:HB2	1.73	0.69
1:B:1541:GLU:OE1	1:B:1555:ARG:HD3	1.94	0.66
1:B:2080:ARG:H	1:B:2081:GLU:HB2	1.59	0.65
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.81	0.63
1:A:2095:ASP:OD2	1:A:2099:ARG:NH1	2.33	0.62
1:A:1494:GLN:HE21	1:A:1496:LYS:H	1.47	0.61
1:C:1898:THR:HG22	3:C:142:HOH:O	2.00	0.61
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.49	0.59
1:B:2080:ARG:N	1:B:2081:GLU:HB2	2.18	0.59
1:B:2164:ASP:H	1:B:2170:GLN:NE2	2.02	0.58
1:A:1900:GLU:HG2	1:A:1918:GLN:HG2	1.85	0.57
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.70	0.57
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.70	0.57
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.68	0.57
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.05	0.56
1:C:1759:ALA:H	1:C:1774:ASN:ND2	2.05	0.55
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.04	0.55
1:A:1759:ALA:H	1:A:1774:ASN:ND2	2.05	0.55
1:B:1759:ALA:H	1:B:1774:ASN:ND2	2.05	0.55
1:C:1582:PHE:CD2	1:C:1807:MET:HE1	2.43	0.52
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.06	0.52
1:B:2046:ARG:NH2	1:C:1639:PHE:O	2.43	0.52
1:A:2184:ASP:OD2	1:B:1481:ARG:NH2	2.36	0.51
1:C:1900:GLU:HG2	1:C:1918:GLN:HG2	1.92	0.51
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	1.92	0.51
1:B:1969:LYS:HA	1:C:1741:ARG:HD2	1.93	0.50
1:C:2030:THR:HG21	3:C:955:HOH:O	2.10	0.49
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.42	0.49
1:B:2183:ASP:O	1:B:2187:LYS:HG2	2.12	0.49
1:B:1582:PHE:CD2	1:B:1807:MET:HE1	2.48	0.49
1:A:2033:ILE:HG22	1:A:2034:LYS:HG2	1.95	0.49
1:B:1852:THR:HG22	1:B:1855:GLY:O	2.13	0.49
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.46	0.49
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.13	0.49
1:A:1813:LYS:HE2	1:A:1816:MET:HE3	1.94	0.48
1:A:1846:MET:HE1	1:A:1990:PRO:HB2	1.95	0.48
1:C:2044:MET:HE1	1:C:2083:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2138:ARG:NH2	1:C:2183:ASP:OD1	2.47	0.48
1:C:1623:ALA:HA	1:C:1730:CYS:HB3	1.96	0.48
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.79	0.48
1:C:1846:MET:HE1	1:C:1990:PRO:HB2	1.95	0.47
1:A:2142:GLN:O	1:A:2142:GLN:HG2	2.13	0.47
1:C:1499:LYS:O	1:C:1503:MET:HG2	2.15	0.47
1:C:1606:LYS:HD2	3:C:967:HOH:O	2.15	0.47
1:A:2031:VAL:HG13	1:A:2035:PHE:HB3	1.98	0.46
1:B:2034:LYS:HD2	1:C:1630:GLY:HA2	1.98	0.46
1:B:2044:MET:HE1	1:B:2083:LEU:HD12	1.98	0.46
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.16	0.45
1:A:1877:VAL:CG2	1:A:1928:SER:HB2	2.43	0.45
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.13	0.45
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.98	0.45
1:C:1753:PRO:HB3	1:C:1775:LEU:HD13	1.99	0.44
1:B:1639:PHE:O	1:C:2046:ARG:NH2	2.50	0.44
1:A:1818:VAL:HB	1:A:1888:PRO:HG2	2.00	0.44
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.65	0.44
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.65	0.44
1:B:1606:LYS:HE3	1:B:1606:LYS:HB2	1.71	0.44
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.00	0.44
1:B:1480:LEU:HA	1:B:1492:TRP:CD1	2.53	0.43
1:B:1954:ARG:O	1:B:1996:ARG:HB2	2.18	0.43
1:A:1544:GLU:OE2	1:A:1602:GLU:OE1	2.37	0.43
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.01	0.43
1:C:2142:GLN:H	1:C:2142:GLN:HG2	1.73	0.43
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.17	0.42
1:B:1909:ASN:HD22	1:B:1910:PRO:HD2	1.84	0.42
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.66	0.42
1:B:1523:TRP:HB3	1:B:1530:VAL:HG11	2.01	0.42
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.19	0.42
1:B:2086:TYR:HA	1:B:2089:ILE:HD12	2.01	0.42
1:A:1883[B]:ARG:NH1	1:A:1886:GLY:O	2.51	0.41
1:C:1655:TYR:CE1	1:C:1689:VAL:HG22	2.55	0.41
1:C:1762:LEU:HD12	1:C:1762:LEU:HA	1.92	0.41
1:A:2099:ARG:NH2	3:A:447:HOH:O	2.53	0.41
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.85	0.41
1:B:2093:PHE:O	1:B:2097:HIS:HD2	2.03	0.41
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.51	0.41
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.21	0.41
1:B:1544:GLU:OE2	1:B:1602:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.50	0.41
1:C:1544:GLU:OE2	1:C:1602:GLU:OE1	2.38	0.41
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.50	0.41
1:C:2097:HIS:O	1:C:2102:ARG:HG3	2.20	0.41
1:C:1954:ARG:O	1:C:1996:ARG:HB2	2.21	0.41
1:A:1582:PHE:CD2	1:A:1807:MET:HE1	2.56	0.41
1:A:2037:ARG:HG2	3:A:91:HOH:O	2.20	0.41
1:A:2093:PHE:O	1:A:2097:HIS:HD2	2.04	0.41
1:B:1481:ARG:HA	1:B:1482:PRO:HA	1.95	0.41
1:C:2093:PHE:O	1:C:2097:HIS:HD2	2.04	0.41
1:B:1781:GLN:NE2	1:B:1781:GLN:H	2.19	0.40
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.57	0.40
1:A:1901:ASN:ND2	3:A:960:HOH:O	2.53	0.40
1:C:1909:ASN:HD22	1:C:1910:PRO:HD2	1.85	0.40
1:A:1909:ASN:HD22	1:A:1910:PRO:HD2	1.85	0.40
1:B:2164:ASP:H	1:B:2170:GLN:HE22	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	693/769 (90%)	670 (97%)	21 (3%)	2 (0%)	36	50
1	B	686/769 (89%)	658 (96%)	23 (3%)	5 (1%)	18	28
1	C	677/769 (88%)	651 (96%)	20 (3%)	6 (1%)	14	22
All	All	2056/2307 (89%)	1979 (96%)	64 (3%)	13 (1%)	21	32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2081	GLU

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Mol	Chain	Res	Type
1	C	2144	GLY
1	A	1997	GLY
1	A	2143	VAL
1	B	1997	GLY
1	B	2046	ARG
1	B	2145	GLU
1	C	1997	GLY
1	C	2046	ARG
1	C	2080	ARG
1	C	2081	GLU
1	C	2145	GLU
1	B	1481	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/658 (90%)	557 (94%)	34 (6%)	18	32
1	B	586/658 (89%)	546 (93%)	40 (7%)	14	25
1	C	578/658 (88%)	535 (93%)	43 (7%)	13	22
All	All	1755/1974 (89%)	1638 (93%)	117 (7%)	15	26

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1524	LYS
1	A	1585	VAL
1	A	1602	GLU
1	A	1606	LYS
1	A	1618	ARG
1	A	1629	ILE
1	A	1641	VAL
1	A	1666	LEU
1	A	1673	ASN
1	A	1676	LEU

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Mol	Chain	Res	Type
1	A	1682	ILE
1	A	1687	ARG
1	A	1691	LYS
1	A	1700	LEU
1	A	1732	SER
1	A	1756	LEU
1	A	1766	LEU
1	A	1781	GLN
1	A	1826	THR
1	A	1879	VAL
1	A	1915	THR
1	A	1924	TRP
1	A	1950	LEU
1	A	2002	VAL
1	A	2003	VAL
1	A	2038	GLU
1	A	2047	LEU
1	A	2078	ARG
1	A	2083	LEU
1	A	2139	LEU
1	A	2142	GLN
1	A	2148	ARG
1	A	2190	LYS
1	A	2191	LEU
1	B	1480	LEU
1	B	1483	ILE
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1524	LYS
1	B	1555	ARG
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1618	ARG
1	B	1629	ILE
1	B	1666	LEU
1	B	1673	ASN
1	B	1679	ARG
1	B	1686	GLU
1	B	1689	VAL
1	B	1762	LEU

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Mol	Chain	Res	Type
1	B	1781	GLN
1	B	1824	LYS
1	B	1839	GLU
1	B	1843	VAL
1	B	1852	THR
1	B	1924	TRP
1	B	2001	VAL
1	B	2025	LEU
1	B	2033	ILE
1	B	2038	GLU
1	B	2040	LEU
1	B	2077	ASP
1	B	2083	LEU
1	B	2116	THR
1	B	2142	GLN
1	B	2145	GLU
1	B	2148	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2180	LYS
1	B	2183	ASP
1	B	2189	LEU
1	C	1508	VAL
1	C	1524	LYS
1	C	1550	LEU
1	C	1585	VAL
1	C	1602	GLU
1	C	1606	LYS
1	C	1618	ARG
1	C	1654	GLN
1	C	1666	LEU
1	C	1673	ASN
1	C	1680	THR
1	C	1731	ARG
1	C	1740	VAL
1	C	1741	ARG
1	C	1762	LEU
1	C	1770	VAL
1	C	1781	GLN
1	C	1792	THR
1	C	1824	LYS
1	C	1838	ASP

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Mol	Chain	Res	Type
1	C	1839	GLU
1	C	1879	VAL
1	C	1901	ASN
1	C	1902	LEU
1	C	1915	THR
1	C	1924	TRP
1	C	1950	LEU
1	C	2001	VAL
1	C	2030	THR
1	C	2033	ILE
1	C	2034	LYS
1	C	2038	GLU
1	C	2047	LEU
1	C	2055	ARG
1	C	2079	GLU
1	C	2083	LEU
1	C	2102	ARG
1	C	2114	GLU
1	C	2142	GLN
1	C	2152	ILE
1	C	2186	LEU
1	C	2190	LYS
1	C	2192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1581	GLN
1	A	1587	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1763	ASN
1	A	1774	ASN
1	A	1781	GLN
1	A	1815	ASN
1	A	1837	ASN
1	A	1934	GLN
1	A	1944	GLN
1	A	2011	GLN
1	A	2097	HIS
1	A	2165	HIS

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Mol	Chain	Res	Type
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1581	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1654	GLN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1781	GLN
1	B	1815	ASN
1	B	1918	GLN
1	B	1934	GLN
1	B	1944	GLN
1	B	2008	ASN
1	B	2092	GLN
1	B	2097	HIS
1	B	2170	GLN
1	C	1517	GLN
1	C	1581	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1748	GLN
1	C	1752	GLN
1	C	1763	ASN
1	C	1774	ASN
1	C	1781	GLN
1	C	1815	ASN
1	C	1837	ASN
1	C	1901	ASN
1	C	1922	GLN
1	C	1944	GLN
1	C	2011	GLN
1	C	2045	ASN
1	C	2092	GLN
1	C	2097	HIS
1	C	2142	GLN
1	C	2165	HIS
1	C	2170	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	B37	B	2242	-	41,41,41	1.19	1 (2%)	56,58,58	1.12	3 (5%)
2	B37	C	2242	-	41,41,41	1.18	4 (9%)	56,58,58	1.17	4 (7%)
2	B37	A	2242	-	41,41,41	1.28	5 (12%)	56,58,58	1.21	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B37	B	2242	-	-	0/16/26/26	0/6/6/6
2	B37	C	2242	-	-	0/16/26/26	0/6/6/6
2	B37	A	2242	-	-	0/16/26/26	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2242	B37	C54-C43	-3.40	1.43	1.49
2	C	2242	B37	C54-C43	-3.06	1.44	1.49
2	B	2242	B37	C54-C43	-2.95	1.44	1.49
2	C	2242	B37	C38-N26	2.28	1.39	1.34
2	A	2242	B37	C38-N26	2.19	1.39	1.34
2	C	2242	B37	C39-C40	-2.18	1.38	1.42
2	A	2242	B37	C39-C40	-2.17	1.38	1.42
2	A	2242	B37	C40-C41	-2.12	1.39	1.42
2	C	2242	B37	C49-C41	-2.10	1.38	1.41
2	A	2242	B37	C27-N26	-2.04	1.43	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2242	B37	C39-C44-C43	-2.89	117.37	120.63
2	B	2242	B37	C39-C44-C43	-2.83	117.43	120.63
2	C	2242	B37	C9-C3-C4	2.77	121.85	118.31
2	A	2242	B37	C9-C3-C4	2.69	121.75	118.31
2	B	2242	B37	C27-N26-C25	2.40	117.58	112.68
2	A	2242	B37	O65-C38-N26	2.27	125.93	122.35
2	C	2242	B37	C39-C44-C43	-2.21	118.13	120.63
2	A	2242	B37	C28-C27-N26	-2.16	106.43	110.66
2	C	2242	B37	C27-N26-C25	2.08	116.92	112.68
2	B	2242	B37	O65-C38-C39	-2.07	116.19	120.47
2	A	2242	B37	C46-C40-C41	2.06	120.64	118.36
2	C	2242	B37	C12-C4-N5	2.03	121.66	118.69
2	A	2242	B37	C44-C43-N42	2.02	124.01	122.17

There are no chirality outliers.

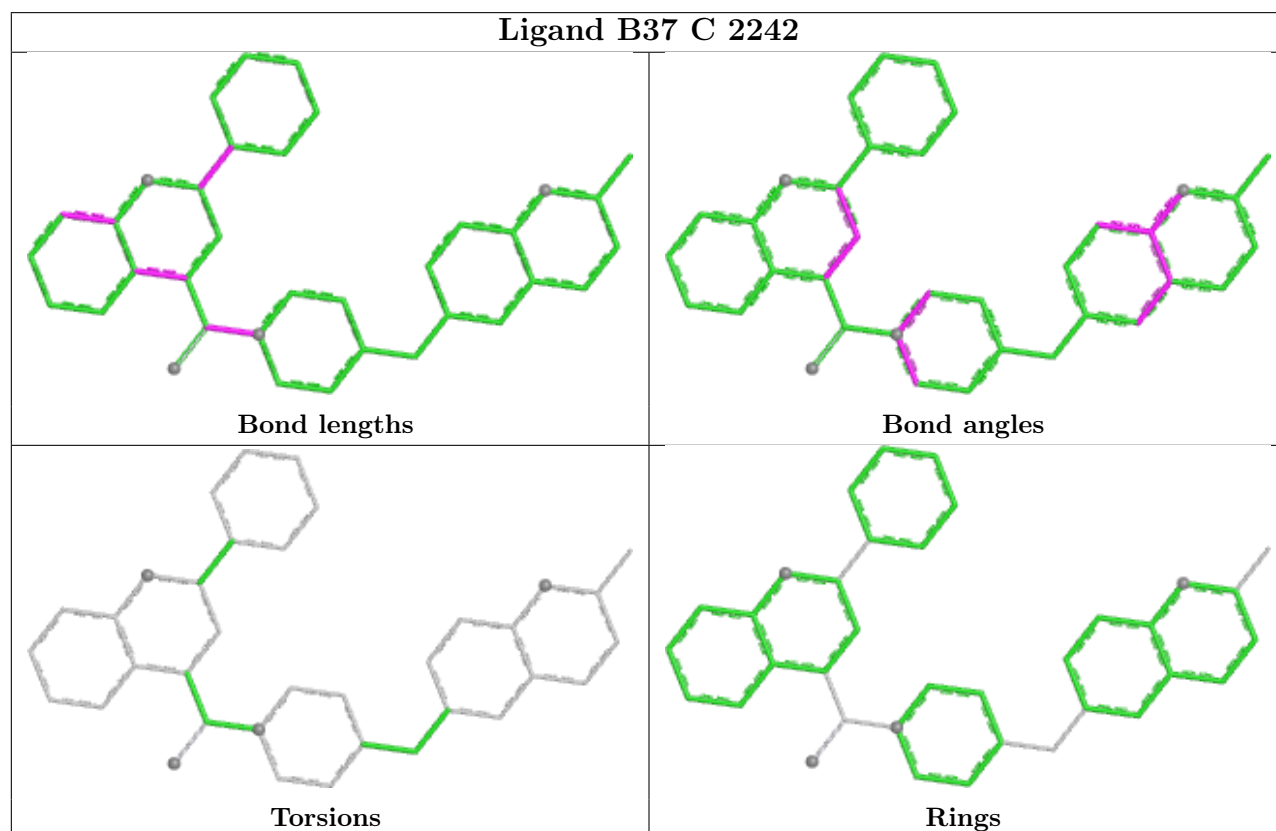
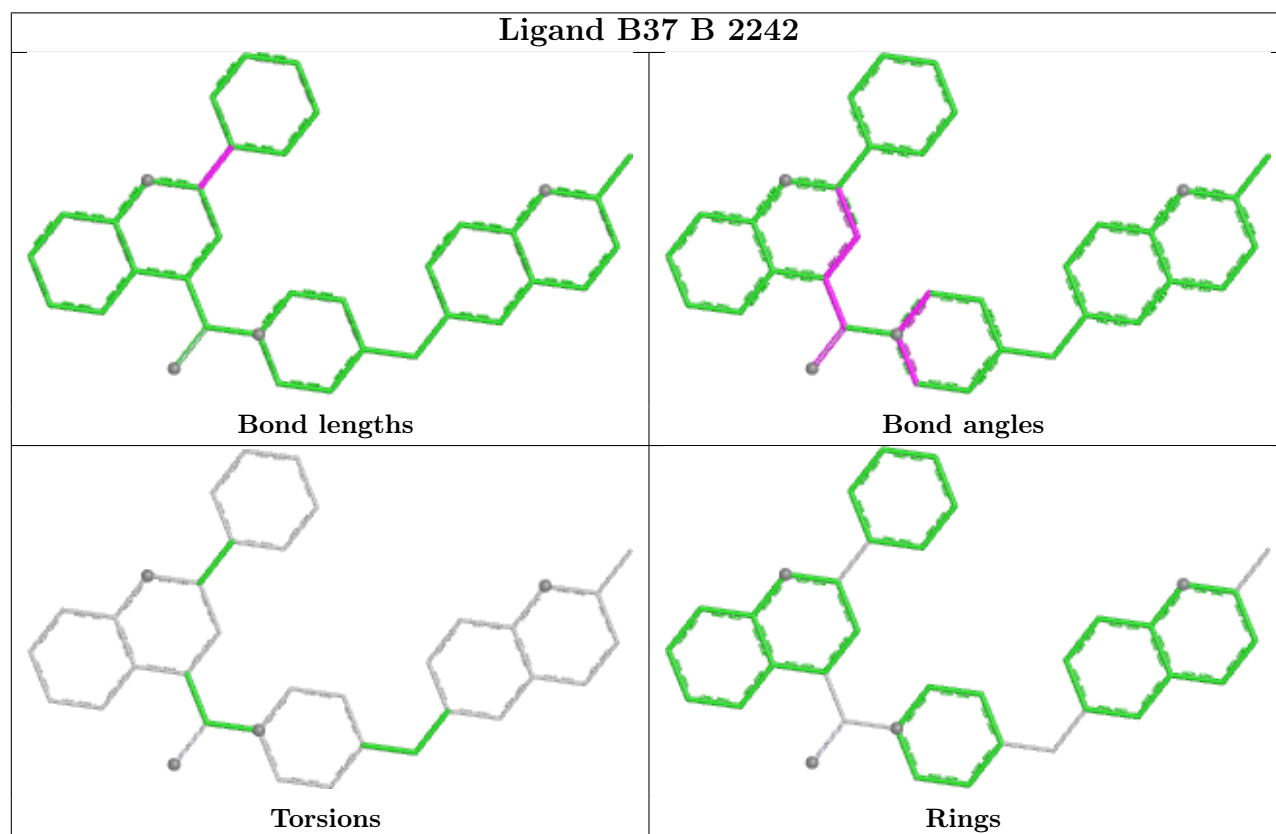
There are no torsion outliers.

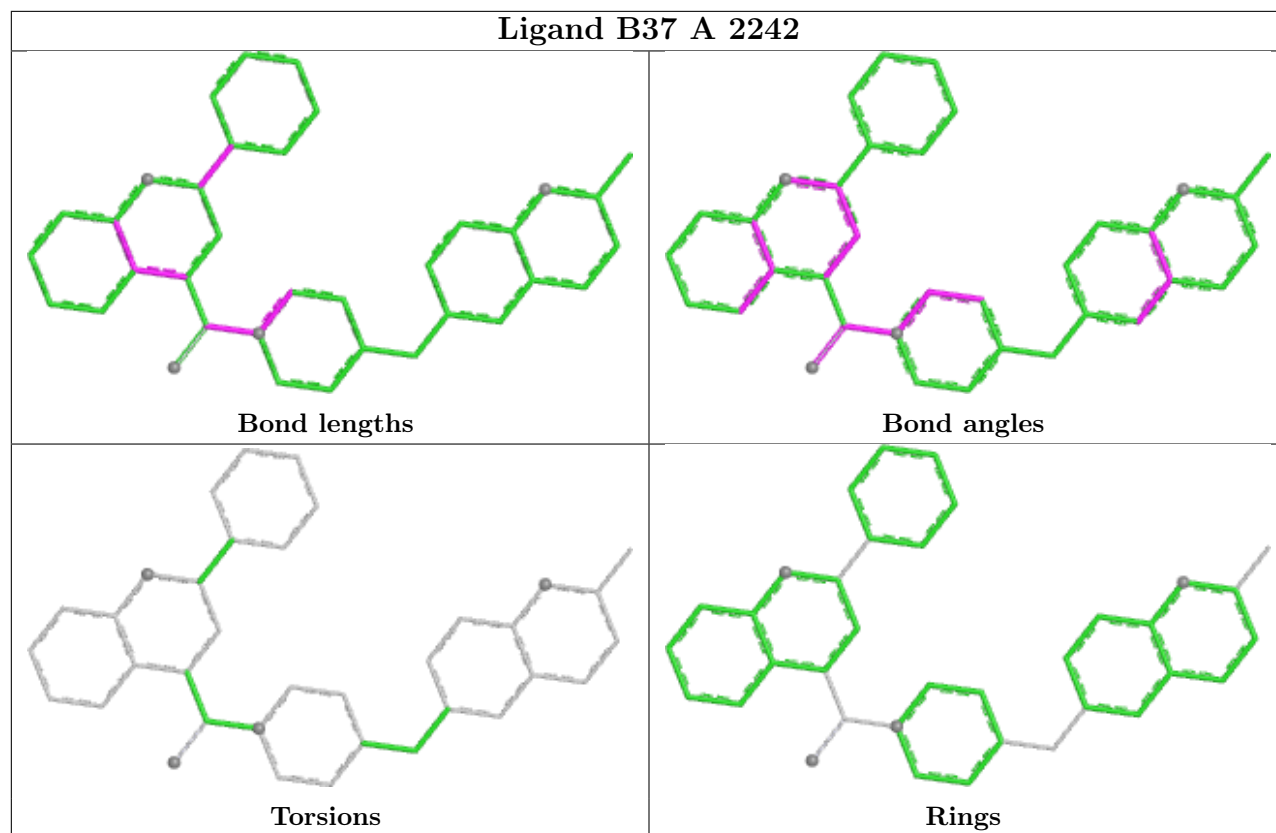
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	696/769 (90%)	0.09	28 (4%)	42	38	32, 56, 111, 147	1 (0%)
1	B	690/769 (89%)	0.22	42 (6%)	27	23	40, 61, 119, 159	0
1	C	681/769 (88%)	0.15	34 (4%)	34	30	38, 59, 123, 153	0
All	All	2067/2307 (89%)	0.15	104 (5%)	34	30	32, 58, 118, 159	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2189	LEU	8.4
1	B	2179	TYR	6.3
1	A	2195	ALA	6.2
1	C	2143	VAL	6.2
1	B	2054	LEU	6.1
1	A	2143	VAL	5.4
1	A	2144	GLY	5.1
1	A	2191	LEU	5.0
1	A	2194	PHE	4.5
1	B	1681	VAL	4.3
1	B	2075	LEU	4.3
1	B	2134	TYR	4.3
1	C	2144	GLY	4.1
1	B	1480	LEU	3.8
1	C	2192	GLU	3.8
1	A	2073	LYS	3.7
1	A	2190	LYS	3.5
1	C	2057	GLN	3.4
1	C	1682	ILE	3.4
1	B	1824	LYS	3.3
1	A	2142	GLN	3.2
1	A	1680	THR	3.2
1	B	2085	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	2191	LEU	3.1
1	C	2075	LEU	3.0
1	C	1643	TRP	3.0
1	B	1839	GLU	3.0
1	C	2141	HIS	2.9
1	A	2148	ARG	2.9
1	B	1918	GLN	2.9
1	B	1683	ASN	2.9
1	A	2193	SER	2.8
1	A	1911	ASN	2.8
1	B	2082	LEU	2.8
1	B	2083	LEU	2.8
1	A	1650	ASP	2.8
1	B	2050	LYS	2.7
1	B	1682	ILE	2.7
1	A	2050	LYS	2.7
1	A	2141	HIS	2.6
1	A	1668	LYS	2.6
1	B	2149	LEU	2.6
1	A	1682	ILE	2.6
1	B	1483	ILE	2.6
1	A	2192	GLU	2.6
1	B	2142	GLN	2.5
1	A	1647	ALA	2.5
1	C	2190	LYS	2.5
1	C	2055	ARG	2.5
1	A	1524	LYS	2.5
1	C	1679	ARG	2.5
1	A	2149	LEU	2.5
1	C	2054	LEU	2.5
1	A	2052	ARG	2.5
1	C	2053	GLU	2.5
1	B	1531	LYS	2.5
1	C	1669	PHE	2.5
1	B	2143	VAL	2.5
1	B	1647	ALA	2.5
1	B	2188	GLY	2.4
1	B	2167	ASP	2.4
1	C	1647	ALA	2.4
1	A	1531	LYS	2.4
1	C	1649	PRO	2.4
1	C	1684	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2077	ASP	2.4
1	B	2086	TYR	2.4
1	B	2181	THR	2.3
1	B	1530	VAL	2.3
1	C	1651	LYS	2.3
1	A	2037	ARG	2.3
1	C	1652	GLY	2.3
1	B	1649	PRO	2.3
1	C	1773	SER	2.3
1	B	1651	LYS	2.3
1	A	1530	VAL	2.3
1	A	1649	PRO	2.3
1	B	2186	LEU	2.3
1	B	2144	GLY	2.2
1	C	2080	ARG	2.2
1	B	2045	ASN	2.2
1	C	1530	VAL	2.2
1	B	2041	LEU	2.2
1	C	2114	GLU	2.2
1	C	1668	LYS	2.2
1	B	2141	HIS	2.2
1	C	2045	ASN	2.2
1	A	1669	PHE	2.2
1	B	1669	PHE	2.2
1	C	2076	ALA	2.1
1	B	2037	ARG	2.1
1	B	2182	LEU	2.1
1	C	1656	LEU	2.1
1	C	1680	THR	2.1
1	C	1852	THR	2.1
1	C	1816	MET	2.1
1	B	2080	ARG	2.1
1	B	1629	ILE	2.1
1	C	1681	VAL	2.1
1	C	1524	LYS	2.1
1	C	2046	ARG	2.0
1	B	2145	GLU	2.0
1	A	1651	LYS	2.0
1	B	1840	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

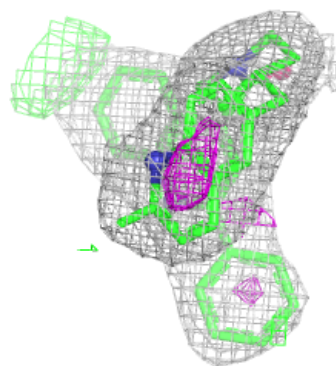
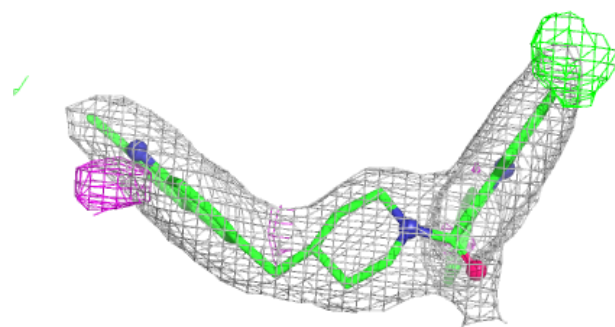
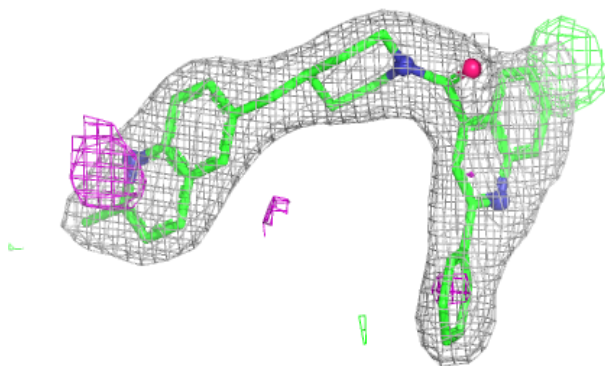
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B37	B	2242	36/36	0.93	0.12	59,67,82,84	0
2	B37	A	2242	36/36	0.94	0.11	49,55,77,79	0
2	B37	C	2242	36/36	0.95	0.10	51,60,76,77	0

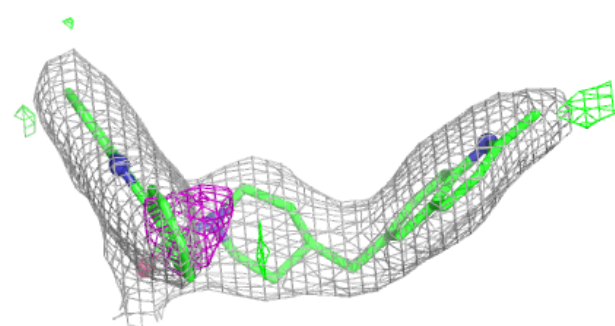
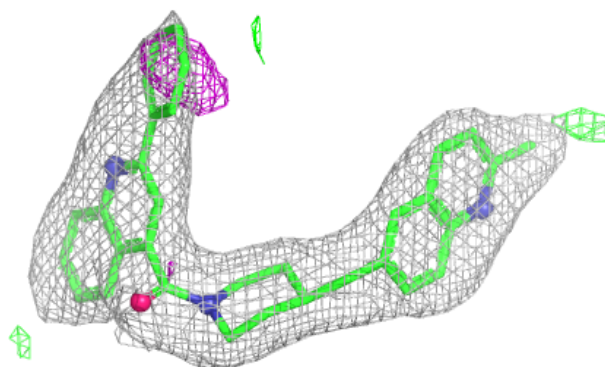
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B37 B 2242:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

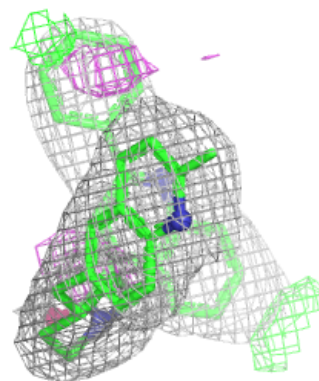
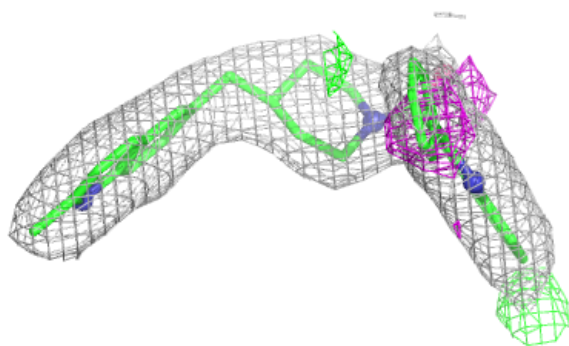
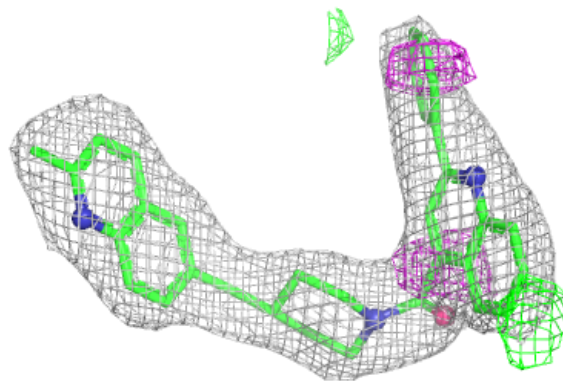
**Electron density around B37 A 2242:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B37 C 2242:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.